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Differential equation for spectral flows of hermitean Wilson-Dirac operator

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Abstract

Establishing an exact relation for the derivative we show that the eigenvalue flows of the hermitean Wilson-Dirac operator obey a differential equation. We obtain a complete overview of the characteristic features of its solutions. The underlying mathematical aspects are fully clarified.

1. Introduction

The hermitean Wilson-Dirac operator H is a fundamental quantity in the overlap formalism [1, 2]. It has been shown there that the difference of the numbers of its positive and negative eigenvalues is related to the index of the massless Dirac operator. This gets particularly explicit with the Neuberger operator [3].

The consideration of eigenvalue flows of H introduced in [2] has initiated a number of numerical works on such flows, including studies of the index theorem [4], of topological susceptibility [5], of instanton effects [6], and of the spectrum gap with the mass parameter [7]. In these works the derivative of the flows has been used [4, 6], considering the respective relation as a result of first-order perturbation theory [4]. In theoretical considerations of these flows, as in Section 8 of Ref. [2], details of the behavior at crossing have been of interest. Further, questions concerning the eigenvalue flows have also been raised in investigations [8, 9] of the vicinities of the parameter values $-m/r = 0, 2, 4, 6, 8$.

Generally one should be aware of the fact that the considerations of eigenvalue flows of H actually imply certain smoothness conditions to hold, which goes beyond the solving of

the eigenvalue equation at individual points. Locally this requires adequate properties of derivatives and globally that integration provides appropriate solutions. In the case of the specific hermitean operator considered, in unitary space fortunately there are theorems [10] which we can use to settle the first point. To clarify the second point we have to develop an appropriate procedure of integration.

In the present paper we derive a differential equation for the eigenvalues of the hermitean Wilson-Dirac operator H and give a complete specification of its admissible solutions. We are able to do this in a mathematically well defined way.

Our developments appear important for a number of problems. In particular, there is the ambiguity in the choice of the mass parameter m which affects the counting of crossings of flows on a finite lattice. So far, from an upper bound on the gauge field, a bounding function has been derived [9] which e.g. allows to disentangle physical and doubler regions. One can hope that the differential-equation properties found here allow to extract more detailed information within this respect. In a study of the locality [11] of the Neuberger operator [3] a lower bound for H^2, also relying on the above gauge-field bound, has been important. In such investigations again the differential equation may help to get sharper results. In present Monte-Carlo simulations with massless quarks (with overlap as well as with domain wall fermions) there are severe problems due to too small values occurring for H^2 [12]. The proposals to deal with this include projecting out some subspace of small eigenvalues of H [13], constructing forms of H which are better behaved around zero [14], and looking for more suitably gauge-field actions [12]. There are now hopes that the differential equation, allowing a more detailed insight, may guide to a way out of these difficulties. Studying flows numerically one generally has to interpolate between a finite number of points. It appears possible to develop more efficient methods for this which use the general properties obtained for the differential-equation solutions.

In the following we first derive the differential equation for the eigenvalue flows of H (Section 2). We then discuss the mathematical properties involved and restrictions due to the eigenequation (Section 3). Next we integrate the differential equation and give a complete overview of its admissible solutions (Section 4). Finally we collect some conclusions (Section 5).

2. Derivation of differential equation

The Wilson-Dirac operator X/a is given by

$$X = \frac{r}{2}\sum_\mu \nabla_\mu^\dagger \nabla_\mu + m + \frac{1}{2}\sum_\mu \gamma_\mu(\nabla_\mu - \nabla_\mu^\dagger) \tag{2.1}$$

where $(\nabla_\mu)_{n'n} = \delta_{n'n} - U_{\mu n}\delta_{n',n+\hat\mu}$ and $0 < r \le 1$. Its property $X^\dagger = \gamma_5 X \gamma_5$ implies that

$$H = \gamma_5 X \tag{2.2}$$

is hermitean. The operator H has the eigenequation

$$H\phi_l = \alpha_l \phi_l \tag{2.3}$$

where α_l is real and the ϕ_l form a complete orthonormal set in unitary space, as one has on a finite lattice.

Multiplying (2.3) by $\phi_l^\dagger \gamma_5$ one gets $\phi_l^\dagger \gamma_5 H \phi_l = \alpha_l \phi_l^\dagger \gamma_5 \phi_l$ and summing this and its hermitian conjugate one has $\phi_l^\dagger \{\gamma_5, H\} \phi_l = 2\alpha_l \phi_l^\dagger \gamma_5 \phi_l$. From this by inserting (2.2) with (2.1) one obtains

$$\alpha_l \, \phi_l^\dagger \gamma_5 \phi_l = m + g_l(m) \tag{2.4}$$

where

$$g_l(m) = \frac{r}{2} \sum_\mu ||\nabla_\mu \phi_l||^2 \; . \tag{2.5}$$

For $g_l(m)$ using $||\nabla_\mu \phi_l|| \le ||(\nabla_\mu - 1\!\!1)\phi_l|| + ||\phi_l|| = 2$ one gets

$$0 \le g_l(m) \le 8r \; . \tag{2.6}$$

Further, abbreviating $(\mathrm{d}\,\alpha_l)/(\mathrm{d}\,m)$ by $\dot{\alpha}_l$, we obtain

$$\frac{\mathrm{d}\,(\phi_l^\dagger H \phi_l)}{\mathrm{d}\,m} = \phi_l^\dagger \dot{H} \phi_l + \dot{\phi}_l^\dagger H \phi_l + \phi_l^\dagger H \dot{\phi}_l = \phi_l^\dagger \gamma_5 \phi_l + \alpha_l \frac{\mathrm{d}\,(\phi_l^\dagger \phi_l)}{\mathrm{d}\,m} \tag{2.7}$$

which means that we have

$$\dot{\alpha}_l = \phi_l^\dagger \gamma_5 \phi_l \; . \tag{2.8}$$

Combining (2.4) and (2.8) we get the differential equation

$$\dot{\alpha}_l(m) \alpha_l(m) = m + g_l(m) \tag{2.9}$$

for the eigenvalue flows of the hermitean Wilson-Dirac operator H.

3. Requirements for solutions

In Section 2 actually only continuity of $\phi_l(m)$ would have been needed, which can be seen repeating the calculations of (2.7) in terms of finite differences. In Section 4, analyzing properties of solutions, we shall need $\dot{g}_l(m)$ (at least at certain points) which by (2.5) implies also the existence of $\dot{\phi}_l(m)$. All of this is, however, no problem because in the case considered we have derivatives of $\phi_l(m)$ up to any order. This follows because for our hermitean operator of form $H(m) = H(0) + m\gamma_5$ in unitary space theorems [10] apply by which $\phi_l(m)$ gets holomorphic on the real axis.

Of the (continuously) infinite number of solutions of (2.9), specified by integration constants, only a discrete finite subset occurs for a given H, the selection depending on H.

The number of solutions in this subset, being the number of eigenvectors of H, is simply the dimension of the unitary space.

Because of (2.8) by the continuity of $\phi_l(m)$ also $\dot{\alpha}_l(m)$ must be continuous for all m in order that the respective solution $\alpha_l(m)$ of (2.9) belongs to the admissible subset. Since the eigenvectors $\phi_l(m)$ have derivatives up to any order this must also hold for the admissible $\alpha_l(m)$. Because of the continuity required for admissible $\alpha_l(m)$ only solutions of the differential equation (2.9) are admitted which exist for all m.

4. Solutions of differential equation

Instead of (2.9) we first consider the differential equation

$$\dot{\beta}_l(m) = 2(m + g_l(m)) \tag{4.1}$$

which by inserting $\beta_l(m) = \alpha_l^2(m)$ becomes (2.9). Integration of (4.1) readily gives

$$\beta_l(m) = \beta_l(m_b) + 2\int_{m_b}^{m} \mathrm{d}\, m'(m' + g_l(m')) \tag{4.2}$$

in which particular solutions are determined by the choices of m_b and $\beta_l(m_b)$. These choices are restricted here by the fact that one actually wants real solutions of (2.9) which meet the requirements discussed in Section 3.

To get an overview of the properties of (4.2) we note that

$$\int_{\hat{m}}^{m} \mathrm{d}\, m'(m' + g_l(m'))\ , \tag{4.3}$$

where $\hat{m}$ is an arbitrarily fixed value, has a minimum at $m = m_y$ if

$$m_y + g_l(m_y) = 0 \quad \text{and} \quad \dot{g}_l(m_y) > -1\ . \tag{4.4}$$

Because of

$$H \to m\gamma_5 \quad \text{for} \quad |m| \to \infty \tag{4.5}$$

one has $\phi_l(m) \to \chi_\pm$ with $\gamma_5\chi_\pm = \pm\chi_\pm$ in this limit. Then in (2.4) one gets $\alpha_l\, \phi_l^\dagger\gamma_5\phi_l \to (\pm m)(\pm 1) = m$ so that one obtains $g_l(m) \to 0$ for $|m| \to \infty$. From this and $g_l(m) \geq 0$ it follows that there is at least one solution $m_y \leq 0$ of (4.4). In general several ones with $m_{y_s} < \ldots < m_{y_1} < m_{y_0} \leq 0$ may occur. If there is only one solution of (4.4) we choose $m_b = m_y$. If there are several ones we put m_b equal to the m_{y_ν} related to the lowest minimum of (4.3) (in case of several degenerate ones picking arbitrarily one of them). In this way we achieve that

$$\int_{m_b}^{m} \mathrm{d}\, m'(m' + g_l(m')) \geq 0 \quad \text{for all} \quad m\ . \tag{4.6}$$

In order to get a real solution $\alpha_l(m)$ of (2.9) which exists for all m, according to (4.6) (which takes the value 0 for $m = m_b$) one has to choose $\beta_l(m_b) \geq 0$ in (4.2). At the points m_{y_ν} with minima of (4.2) where $\beta_l(m_{y_\nu}) > 0$ one then immediately sees that for the solutions of (2.9) one has a minimum of $\alpha_l(m) = +\sqrt{\beta_l(m)}$ and a maximum of $\alpha_l(m) = -\sqrt{\beta_l(m)}$. The points where $\beta_l(m_{y_\nu}) = 0$, i.e. the ones with the lowest minima of (4.2), however, need special consideration. There, to clarify the details at crossing, one has (1) to check whether the derivative $\dot{\alpha}_l(m)$ is finite as is necessary in view of (2.8) and (2) to disentangle the solutions related to different signs of the square root properly.

To check under which conditions the derivative $\dot{\alpha}(m)$ remains finite we note that from (2.9) one gets

$$\dot{\alpha}_l^2 = \frac{(m + g_l(m))^2}{\beta_l(m)} \tag{4.7}$$

showing that in case of $\beta_l(\tilde{m}) = 0$ for some $\tilde{m}$ one must also have $\tilde{m} + g_l(\tilde{m}) = 0$ in order that the derivative remains finite. With these relations holding at $\tilde{m}$ one obtains

$$\dot{\alpha}_l^2(m) \to 1 + \dot{g}_l(\tilde{m}) \quad \text{for} \quad m \to \tilde{m}\ . \tag{4.8}$$

Because at the points with $\beta_l(m_{y_\nu}) = 0$ envisaged above (4.4) is satisfied, by (4.8) the existence of the derivative $\dot{\alpha}_l^2(m_{y_\nu})$ at these points with $\alpha_l(m_{y_\nu}) = 0$ is guaranteed. Further, since in (4.4) one has $\dot{g}_l(m_{y_\nu}) > -1$ it follows that $\dot{\alpha}_l^2(m_{y_\nu}) > 0$ there. Thus, because $\dot{\alpha}_l(m)$ should be continuous (as pointed out in Section 3), there must be a crossing point of two solutions $\alpha_l(m)$, i.e. the solutions $\mp\sqrt{\beta_l(m)}$ from below must continue as $\pm\sqrt{\beta_l(m)}$ above the zero and have the derivatives

$$\dot{\alpha}_l(m_{y_\nu}) = \pm\sqrt{1 + \dot{g}_l(m_{y_\nu})} \neq 0 \tag{4.9}$$

at the crossing point.

The asymptotic behavior $\beta_l(m) \to m^2$ for $|m| \to \infty$, which implies $\alpha(m) \to \pm m$, should be obvious from (4.5). If desired it can readily be worked out in more detail estimating the integral in the form

$$\beta_l(m) = \beta_l(m_b) + m^2 - m_b^2 + 2\int_{m_b}^{m} \mathrm{d}\, m' g_l(m') \tag{4.10}$$

of (4.2), which already works using the bound (2.6).

5. Conclusions

Establishing an exact relation for the derivatives of the eigenvalues of the hermitean Wilson-Dirac operator H we have derived a differential equation for the eigenvalue flows

of H. Referring to appropriate theorems also the mathematical aspects have been fully clarified. Unambiguous prescriptions for the selection of admissible solutions have been given. Integrating the differential equation and analyzing the features of its solutions a complete overview has been obtained. Our results appear advantageous for future theoretical developments as well as for applications in numerical works.

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